NORTH-HOLLAND

The Distribution of Eigenvalues of Graphs

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ABSTRACT

We show that every limit point of the kth largest eigenvalues of graphs is a limit point of the $(k+1)$th largest eigenvalues, and we find out the smallest limit point of the kth largest eigenvalues and an upper bound of the limit points of the kth smallest eigenvalues. For $k \geq 4$, we prove that there exists a gap beyond the smallest limit point in which no point is the limit point of the kth largest eigenvalues. For the third largest eigenvalues of a graph G with at least three vertices, we obtain that (1) $\lambda_3(G) < -1$ iff $G \cong P_3$; (2) $\lambda_3(G) = -1$ iff G^c is isomorphic to a complete bipartite graph plus isolated vertices: (3) there exist no graphs such that $-1 < \lambda_3(G) < (1-\sqrt{5})/2$. Consequently, if G^c is not a complete bipartite graph plus isolated vertices, $\lambda_3(G) \geq \lambda_3(D_n^*)$, where D_n^* is the complement of the double star $S(1, n-3)$.

1. INTRODUCTION

Generally speaking, we consider only finite graphs without loops or multiple edges. The join $G_1 \vee G_2$ of two graphs G_1 and G_2 is the graph obtained by adding an edge between each vertex in G_1 and each vertex in G_2. Let G^c denote the complement of a graph G, K_n be the complete graph, P_n the path with n vertices, and $K_{m,n}$ the complete bipartite graph.

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Let G be a graph with vertices $v_1, v_2 \ldots, v_n$. The adjacency matrix of a graph G is defined as a (0, 1) matrix $A(G) = (a_{ij})$ such that $a_{ij} = 1$ iff vertices v_i and v_j are adjacent. The characteristic polynomial of G is the characteristic polynomial of its adjacency matrix, denoted by $\chi(G, \lambda)$. Since $A(G)$ is a real symmetric matrix, its eigenvalues must be real. The kth largest eigenvalue $\lambda_k(G)$ of G is the kth largest root of its characteristic polynomial. Let $\lambda'_k(G) = \lambda_{n-k+1}(G)$ be the kth smallest eigenvalue of G. A real number r is said to be the limit point of the kth largest eigenvalues of graphs if there exists a sequence $\{G_n\}$ of graphs such that $\lim_{n\to\infty} \lambda_k(G_n) = r$. Note that we abuse the definition of limit point. Here we don't require $\lambda_k(G_n)$ distinct for different n, so that if $r = \lambda_k(G)$ for some graph G, then r is a limit point of the kth largest eigenvalues of graphs.

The study of the limit points of eigenvalues of graphs was initiated by A. J. Hoffman [8], where he posed the problem of finding the limit points of eigenvalues of graphs and also determined all limit points of the largest eigenvalues less than $\tau^{1/2} + \tau^{-1/2} \approx 2.058171$($\tau$ is the golden mean). In [9] he found all limit points ≥ -2 of least eigenvalues of graphs. By direct construction, J. Shearer [11] extended Hoffman's work to show that every real number $r \geq \tau^{1/2} + \tau^{-1/2}$ is the limit point of the largest eigenvalues of graphs. More recently, M. Doob [6, 7] generalized Shearer's result to prove that every real number $r \geq \tau^{1/2} + \tau^{-1/2}$ is the limit point of the kth largest eigenvalues of graphs and $r \leq -(\tau^{1/2} + \tau^{-1/2})$ is the limit point of the kth smallest eigenvalues of graphs.

From Hoffman and Shear's results, we know all limit points of the largest eigenvalue. But in general the problem is far from being solved. It is not too difficult to prove that the second eigenvalue of a noncomplete multipartite graph is greater than 0 and there does not exist a graph G such that the second largest eigenvalue of G lies in the interval $(-1, 0)$ (see [1]). A natural question is: does there exist a nontrivial gap of limit points of eigenvalues of graphs? The answer is yes. In our previous paper [1], we showed that $0 \leq \lambda_2(G) \leq \frac{1}{3}$ iff $G \cong (K_1 \cup K_2) \vee K^c_{n-3}$. Consequently, we showed that (0, 0.3) is a gap of limit points of the second largest eigenvalues of graphs. In this paper, we first show that every limit point of the kth largest eigenvalues is a limit point of the $(k+1)$th largest eigenvalues. Then we find the smallest limit point of the kth largest eigenvalues and an upper bound of the limit points of the kth smallest eigenvalues. Next we prove that for $k \geq 4$ there exists a gap beyond the smallest limit point in which no point is the limit point of the kth largest eigenvalues. Finally, for the third largest eigenvalue of a graph G with at least three vertices, we obtain that (1) $\lambda_3(G) < -1$ iff $G \cong P_3$; (2) $\lambda_3(G) = -1$ iff G^c is isomorphic to a complete bipartite graph plus isolated vertices; (3) there exist no graphs such that $-1 < \lambda_3(G) < (1 - \sqrt{5})/2$. Consequently, if G^c is not a complete bipartite graph together with some isolated vertices, then $\lambda_3(G) \geq \lambda_3(D^*_n)$, where D^*_n is the complement of the double star $S(1, n-3)$.

2. LEMMAS AND RESULTS

Let L_k be the set of the limit points of the kth largest eigenvalues of graphs, and L'_k be the set of the limit points of the kth smallest eigenvalues of graphs. We have the following observation.

THEOREM 1. *The sequences $\{L_k\}$ and $\{L'_k\}$ are increasing, i.e.,*

$$L_1 \subseteq L_2 \subseteq \cdots \subseteq L_k \subseteq \cdots, \tag{1}$$

$$L'_1 \subseteq L'_2 \subseteq \cdots \subseteq L'_k \subseteq \cdots. \tag{2}$$

PROOF. Let r be a real number, m an integer greater than r^2, and S the star with $m+1$ vertices. The largest eigenvalue of S is $\sqrt{m}$ greater than $|r|$, and the least eigenvalue is $-\sqrt{m}$ less than $-|r|$. Suppose $r \in L_k$; then there exists a sequence $\{G_n\}$ of graphs such that $\lim_{n\to\infty} \lambda_k(G_n) = r$. If $r > 0$, let $H_n = G_n \cup S$; if $r \leq 0$, let $H_n = G_n \cup K_1$. The spectrum of H_n is the union of the spectra of G_n and S. Obviously, $\lambda_{k+1}(H_n) = \lambda_k(G_n)$ and $\lim_{n\to\infty} \lambda_{k+1}(H_n) = \lim_{n\to\infty} \lambda_k(G_n) = r$. Hence, $r \in L_{k+1}$ and $L_k \subseteq L_{k+1}$, i.e., $\{L_k\}$ is increasing.

To prove (2), let $r \in L'_k$ and $\lim_{n\to\infty} \lambda'_k(G_n) = r$. If $r > 0$, let $H_n = G_n \cup K_1$; if $r \leq 0$, let $H_n = G_n \cup S$. Then $\lambda'_{k+1}(H_n) = \lambda'_k(G_n)$ and $\lim_{n\to\infty} \lambda'_{k+1}(H_n) = \lim_{n\to\infty} \lambda'_k(G_n) = r \in L'_{k+1}$. Therefore $L'_k \subseteq L'_{k+1}$. ■

From Theorem 1 and Shear's result, we can obtain Doob's results [6], i.e., $(\tau^{1/2} + \tau^{-1/2}, \infty) \subset L_k$ and $(-\infty, -\tau^{1/2} - \tau^{-1/2}) \subset L'_k$ for each k. Note that L_k does not have an upper bound and L'_k does not have a lower bound. In the sequel, we will prove the existence of the minimum of L_k and of a gap of L_k to the right of the smallest limit point in which no point is a limit point of the kth largest eigenvalues for each k.

Let V' be a subset of vertices of a graph G, and $|V'| = k$. Denote by $G - V'$ the subgraph obtained from G by deleting all vertices in V'. We summarize some basic results [4] in the following lemma, which will be frequently used throughout the paper.

LEMMA 1. *Let G be a graph with n vertices. Then:*

(1) $\lambda_i(G) \geq \lambda_i(G - V') \geq \lambda_{i+k}(G)(1 \leq i \leq n-k)$.

(2) *If G is bipartite, $\lambda_i(G) = -\lambda_{n-i+1}(G)$ for $1 \leq i \leq n$.*

(3) *If H is a proper subgraph of a connected graph G, then $\lambda_1(H) < \lambda_1(G)$. Hence, if H is a subgraph of a bipartite connected graph G, then $\lambda_n(H) \geq \lambda_n(G)$ with equality iff $G \cong H$.*

(4) *G has only one positive eigenvalue iff G is a complete multipartite graph plus isolated vertices.*

LEMMA 2 (The Courant-Weyl inequalities [10]). *Let $\lambda_k(X)$ be the kth largest eigenvalue of a real symmetric matrix X. If A and B are real symmetric matrices of order n and $C = A + B$ then*

$$\lambda_{n-i-j}(C) \geq \lambda_{n-i}(A) + \lambda_{n-j}(B), \tag{3}$$
$$\lambda_{s+t+1}(C) \leq \lambda_{s+1}(A) + \lambda_{t+1}(B), \tag{4}$$

where $0 \leq i, j, s, i+j+1,\ s+t+1 \leq n$.

LEMMA 3. *Let G be a graph with $n \geq 2$ vertices. Then for $k \geq 2$,*

$$\lambda_k(G) + \lambda_{n-k+2}(G^c) \leq -1 \leq \lambda_k(G) + \lambda_{n-k+1}(G^c).$$

In particular, $\lambda_3(G) + \lambda_{n-1}(G^c) \leq -1$.

PROOF. It directly follows from Lemma 2 by taking $A = A(G), B = A(G^c), C$ $A(K_n)$ and letting $i = n-k, j = k-2, s = k-1$, and $t = n-k$. ■

LEMMA 4. *For a graph G with n vertices, there exists a bipartite subgraph H of G such that*

$$\lambda_n(G) \geq \lambda_n(H)$$

with equality if and only if $G \cong H$. Moreover, if $G \ncong H$, let $e \in G$ be an edge not in H; then $\lambda_n(G) \geq \lambda_n(H+e)$.

PROOF. Let $x = (x_1, x_2, \ldots, x_n)$ be the eigenvector corresponding to $\lambda_n(G)$ and $\|x\| = 1$. Let H be the graph obtained from G by deleting all the edges v_iv_j such that $x_ix_j > 0$. Clearly, H is bipartite with bipartition (X, Y), where $X = \{v_i : x_i \geq 0\}$ and $Y\{v_i : x_i < 0\}$. Let $A(H) = a_{ij}(H)$ be the adjacency matrix of H. Then

$$\begin{aligned}\lambda_n(G) &= \sum_{i,j=1}^{n} a_{ij}x_ix_j \geq \sum_{x_ix_j<0} a_{ij}x_ix_j = \sum_{i,j=1}^{n} a_{ij}(H)x_ix_j \\ &\geq \min_{\|x\|=1} \sum_{i,j=1}^{n} a_{ij}(H)x_ix_j = \lambda_n(H).\end{aligned}$$

If $G \ncong H$, then there exists an edge $e = v_iv_j$ of G that does not belong to H. Hence $a_{ij} = 1$ and the corresponding x_i, x_j satisfy that $x_ix_j > 0$. Thus the first inequality in the above is strict, whence $\lambda_n(G) > \lambda_n(H)$. Furthermore, using the same argument as above, we have $\lambda_n(G) \geq \sum_{i,j=1}^{n} a_{ij}\ (H+e)x_ix_j \geq \lambda_n(H+e)$. ■

For any nonnegative integer k, define the set B_k to be

$$B_k = \{\lambda_k(G) : G \text{ is a bipartite graph with } k \text{ vertices}\}.$$

Note that B_k is finite. Obviously the maximum of B_k is 0. The following lemma is due to G. Constantine [2].

LEMMA 5. *For any positive integer h, the minimum of B_{2h} and B_{2h-1} are $-h$ and $-\sqrt{h(h-1)}$, respectively.*

PROOF. Let G be any bipartite graph with bipartition (X, Y) and $|X| = s, |Y| = t, s + t = k$. By Lemma 1(3) and (4),

$$\lambda_k(G) = -\lambda_1(G) \geq -\lambda_1(K_{s,t}) = \lambda_k(K_{s,t})$$

with equality iff $G \cong K_{s,t}$. It is easy to prove that if $k = 2h$, then $\lambda_k(K_{s,t}) = -\sqrt{st}$ has the minimum $-h$; if $k = 2h - 1$, then $\lambda_k(K_{s,t}) = -\sqrt{st}$ has the minimum $-\sqrt{h(h-1)}$. ∎

THEOREM 2. *For each $k \geq 1$:*

(1) *$B_k \subseteq L_k$ and $B_k \not\subseteq L_{k-1}$. Hence $\{L_k\}$ is strictly increasing.*

(2) *If $k = 2h$, then L_k has a minimum $-h$, and L'_k has an upper bound $-1 - \sqrt{h(h+1)}$; if $k = 2h - 1$, then L_k has a minimum $-\sqrt{h(h-1)}$, and L'_k has an upper bound $-1 - h$.*

PROOF. Obviously, $B_k \subseteq L_k$. For any graph G with $n \geq k$ vertices, by Lemma 1, $\lambda_k(G) \geq \lambda_k(F)$, where F is an induced subgraph of G with exactly k vertices. By Lemma 4, there exists a bipartite subgraph H of F such that $\lambda_k(F) \geq \lambda_k(H)$. Therefore the minimum element of L_k is the minimum element of B_k. By Lemma 3, $\lambda_k(F) = \lambda_{n-k+1}(G) \leq -1 - \lambda_{k+1}(G^c)$. Hence part (2) follows from Lemma 5. Since B_k has different minima for distinct k, so does L_k. Hence $B_k \not\subseteq L_{k-1}$. ∎

A bipartite graph H is said to be *equally bipartite* if H has a bipartition (X, Y) such that $|X| = |Y|$. Every connected bipartite graph is uniquely 2-vertex-colorable. In the same sense, H has a unique bipartition (X, Y).

LEMMA 6. *Let H be a connected graph with k vertices, and G a graph with $n \geq k$ vertices. Assume that every induced subgraph of G with k vertices is isomorphic to H. Then:*

(1) *If* $H \cong P_k$ *with* $k \geq 4$, *then* $G \cong P_k$ *or* C_{k+1}.

(2) *If* H *is equally bipartite and is not isomorphic to* K_2, *or to* P_k *with* $k \geq 3$, *then* $G \cong H$.

(3) *If* $H \cong K_{s,s+1}$, *then* $G \cong K_{s,s+1}$ *or* $K_{s+1,s+1}$.

PROOF. First, we claim that G is connected. Otherwise, G has an induced subgraph F with k vertices that is not connected. Hence, $F \not\cong H$. This contradicts the assumption that every induced subgraph of G with k vertices is isomorphic of H.

(1): Assume that $G \not\cong P_k$. Then G has at least $k+1$ vertices. Since every tree with at least $k+1$ vertices has an induced subgraph F with k vertices that is not connected, then G is not a tree. Let $C = (v_1 v_2 \cdots v_t)$ be the smallest cycle in G. If $t \leq k, G$ has an induced subgraph F with k vertices that contains C. If $t \geq k+2$, then we can easily choose k vertices from the cycle C which induce a nonconnected subgraph of G. In both cases, G has an induced subgraph F with k vertices which is not isomorphic to H: a contradiction. Therefore, $t = k+1$. If $n > k+1$, then G has a vertex w which is not on the cycle C but adjacent to a vertex on C. Without loss of generality, let w be adjacent to v_2. Since $k \geq 4$, the subgraph of G induced by $w, v_1, v_2, \ldots, v_{k-1}$ is not isomorphic to P_k. Again this is a contradiction. Hence $n = k+1$ and $G \cong C_{k+1}$.

(2): First, we prove that G must be bipartite. Otherwise, G contains an odd cycle and hence an induced odd cycle $C = (v_1 v_2 \cdots v_{2h+1})$. If $2h+1 \leq k$, then the vertices on C plus $k - 2h - 1$ other vertices induce a nonbipartite subgraph of G. If $2h+1 > k$, then the vertices $v_1, v_2, \ldots, v_k$ induce a subgraph of G that is isomorphic to P_k, whence $H \cong P_k$. In either case, this contradicts the assumptions. Secondly, let (X, Y) be the bipartition of G, and F an induced subgraph with k vertices. By assumption, $F \cong H$. Let (X_1, Y_2) be the bipartition of F, and let $X_1 \subset X$ and $Y_1 \subset Y$. Since H is connected and equally bipartite, then its independence number $\alpha(H)$ is equal to $|X_1| = |Y_1|$. Note that $|X|, |Y| \geq \alpha$. Now we claim $|X| = |Y| = \alpha$. Otherwise, X or Y plus (or minus) some vertices would induce a subgraph F_1 on k vertices and the independence number would be greater than α. Thus, $F_1 \not\cong H$, which is a contradiction. Therefore $X = X_1, Y = Y_1$, and $G \cong H$.

(3): Let $H \cong K_{s,s+1}$. By the same argument as for (2), G must be a bipartite graph with bipartition (X, Y) such that $|X| = |Y|$ is equal to the independence number of H. Hence, $G \cong K_{s,s+1}$ or $K_{s+1,s+1}$. ■

LEMMA 7. *Let* $e = uv$ *be an edge of a graph, let* $C(e)$ *be the collection of cycles containing* e, *and let* $V(Z)$ *denote the set of vertices in the cycle* Z. *Then* *the characteristic polynomial* $\chi(G,\lambda)$ *satisfies*

$$\chi(G,\lambda) = \chi(G-e,\lambda) - \chi(G-u-v,\lambda) - 2\sum_{Z\in C(e)} \chi(G-V(Z),\lambda).$$

LEMMA 8. *Let* e *be an edge of* $K_{s,t}$ *and* $f \in K_t$ *an edge of* $K^c_{s,t} = K_s \cup K_t$. *Then*

(1) $\chi(K_{s,t}-e,\lambda) = \lambda^{s+t-4}[\lambda^4 - (st-1)\lambda^2 + (s-1)(t-1)]$;
(2) $\chi(K_{s,t}+f,\lambda) = \lambda^{s+t-4}[\lambda^4 - (st+1)\lambda^2 - 2s\lambda + s(t-2)]$.

PROOF. Without loss of generality, let $t \geq s$. By Lemma 6, we have

$$\begin{aligned}
\chi(K_{s,t}-e,\lambda) &= \chi(K_{s,t},\lambda) + \chi(K_{s,-1,t-1},\lambda) + 2\sum_{Z\in C(e)} \chi(K_{s,t}-V(Z),\lambda) \\
&= (\lambda^2 - st)\lambda^{s+t-2} + [\lambda^2 - (s-1)(t-1)]\lambda^{s+t-4} \\
&\quad +2\sum_{i=1}^{t-1}\binom{t-1}{i} i! \binom{s-1}{i} i! \\
&\quad \times [\lambda^2 - (s-i-1)(t-i-1)]\lambda^{s+t-2i-4} \\
&= \lambda^{s+t-4}[\lambda^4 - (st-1)\lambda^2 + (s-1)(t-1)]
\end{aligned}$$

and

$$\begin{aligned}
\chi(K_{s,t}+f,\lambda) &= \chi(K_{s,t},\lambda) - \chi(K_{s,t-2},\lambda) - 2\sum_{Z\in C(e)} \chi(K_{s,t}-V(Z),\lambda) \\
&= (\lambda^2 - st)\lambda^{s+t-2} - [\lambda^2 - s(t-2)]\lambda^{s+t-4} \\
&\quad -2\sum_{i=1}^{s-1}\binom{s}{i} i! \binom{t-2}{i-1}(i-1)! \\
&\quad \times [\lambda^2 - (s-i)(t-i-1)]\lambda^{s+t-2i-3} \\
&= \lambda^{s+t-4}[\lambda^4 - (st+1)\lambda^2 - 2s\lambda + s(t-2)].
\end{aligned}$$

■

THEOREM 3. *For each positive integer* $k \geq 4$,

(1) *if* $k = 2h$, *then there does not exist a graph* G *such that*

$$-h < \lambda_k(G) < -\sqrt{h^2-1};$$

(2) *if* $k = 2h+1$, *then there does not exist a graph* G *such that*

$$-\sqrt{h^2+h} < \lambda_k(G) < -\sqrt{h^2+h-2}.$$

PROOF. (1): Let $k = 2h$. Assume that there exists a graph G such that $-h < \lambda_k(G) < -\sqrt{h^2-1}$. Let F be any induced subgraph of G with k vertices. By Lemma 4, there exists a spanning bipartite subgraph H of F such that $\lambda_k(F) \geq \lambda_k(H)$.

If $H \ncong K_{h,h}$, then H is a subgraph of $K_{h,h} - e$ or $K_{s,t}$ where $s \neq t$. By Lemma 1(3),

$$\lambda_k(H) \geq \min\{\lambda_k(K_{h,h}-e), \lambda_k(K_{s,t})\}.$$

Since $s+t = k = 2h$ and $s \neq t$, then

$$\lambda_k(K_{s,t}) = -\sqrt{st} \geq -\sqrt{h^2-1}.$$

By Lemma 8, $\lambda_k(K_{h,h}-e)$ is the smallest root of the equation $\lambda^4 - (h^2-1)\lambda^2 + (h-1)^2 = 0$. Thus

$$\lambda_k(K_{h,h}-e) = -\left(\frac{h^2-1}{2} + \frac{h-1}{2}\sqrt{h^2+2h-3}\right)^{1/2} > -\sqrt{h^2-1}.$$

Therefore

$$\lambda_k(G) \geq \lambda_k(F) \geq \lambda_k(H) \geq -\sqrt{h^2-1}.$$

This is a contradiction. Hence $H \cong K_{h,h}$.

Now we claim that $F \cong K_{h,h}$. Otherwise, by Lemma 4, $\lambda_k(F) \geq \lambda_k(K_{h,h}+e)$. By Lemma 8, $\lambda_k(K_{h,h}+e)$ is the smallest root of the function $g(\lambda) = \lambda^4 - (h^2+1)\lambda^2 - 2h\lambda + h(h-2)$. It is easy to check that $g'(\lambda) = 4\lambda^3 - 2(h^2+1)\lambda - 2h$ and $g''(\lambda) = 12\lambda^2 - 2(h^2+1)$. Consequently, If $\lambda \leq -\sqrt{h^2-1}$, then $g''(\lambda) > 0$ and

$$g'(\lambda) \leq g'\left(-\sqrt{h^2-1}\right) = -2(h^2-3)\sqrt{h^2-1} - 2h < 0.$$

Therefore, $g(\lambda)$ is decreasing on the interval $(-\infty, -\sqrt{h^2-1}]$. Thus If $\lambda \leq -\sqrt{h^2-1}$, then

$$g(\lambda) \geq g\left(-\sqrt{h^2-1}\right) = 2h\sqrt{h^2-1} - h^2 - 2h + 2 > 0.$$

Hence the smallest root of $g(\lambda)$ is greater than $-\sqrt{h^2-1}$. Then

$$\lambda_k(G) \geq \lambda_k(F) \geq \lambda_k(K_{h,h}+e) > -\sqrt{h^2-1}.$$

This is a contradiction. Therefore, every induced graph of G with k vertices is isomorphic to $K_{h,h}$. By Lemma 5(2), $G \cong K_{h,h}$, whence $\lambda_k(G) = -h$. This contradicts $\lambda_k(G) > -h$. Hence, there does not exist a graph G such that

$$-h < \lambda_k(G) < -\sqrt{h^2 - 1}.$$

(2): Let $k = 2h + 1$. Suppose there exists a graph G such that $-\sqrt{h^2 + h} < \lambda_k(G) < -\sqrt{h^2 + h - 2}$. Similiarly, we can prove that every induced graph of G with k vertices is isomorphic to $K_{h,h+1}$. By Lemma 5(3), $G \cong K_{h+1,h+1}$ or $K_{h,h+1}$. Hence

$$\lambda_k(G) = 0 \text{ or } -\sqrt{h^2 + h}.$$

This is a contradiction, and part (2) is proved. ∎

From the above proof of Theorem 3, we can easily obtain the second and third least limit points of the kth largest eigenvalues for $k \geq 4$. Hence the interval between the second and third least limit points is another gap in which no point does not belongs to L_k. However, for any real number r, we conjecture that r is the limit point of the kth eigenvalue of graphs for sufficiently large k:

CONJECTURE 1. Let R be the set of all real numbers. Then

$$\lim_{k \to \infty} L_k = R \quad \text{and} \quad \lim_{k \to \infty} L'_k = R.$$

3. THE THIRD LARGEST EIGENVALUE

Note that Theorem 3 just deals with the kth largest eigenvalues for $k \geq 4$. When $k = 1$ or 2, Theorem 3 is trivial; when $k = 3$, Theorem 3 does not hold. The second largest eigenvalue has been considered in [1]. In this section, we will consider the third largest eigenvalue. The eigenvalues of a graph with order ≤ 5 will be frequently used and can be found in [4].

LEMMA 9. *For every graph G with at least four vertices,*

$$\lambda_3(G) \geq -1.$$

Moreover, if G^c is not bipartite,

$$\lambda_3(G) \geq 0.$$

PROOF. Let V' be a subset of vertices of G and $|V'| = n - 4$. Since every graph on four vertices has the third largest eigenvalue ≥ -1, by Lemma 1(1) we have

$$\lambda_3(G) \geq \lambda_3(G - V') \geq -1.$$

If G^c is not bipartite, G^c contains an odd cycle. Let C_{2k+1} be an odd cycle in G^c with the smallest length. C_{2k+1} must be an induced subgraph of G^c. If $k = 1$ then $\lambda_3(G) \geq \lambda_3(K_3^c) = 0$; if $k = 2$ then $\lambda_3(G) \geq \lambda_3(C_5^c) = \lambda_3(C_5) - 0.6180 > 0$. Let $k \geq 3$. G^c contains P_5, as an induced subgraph, whence G contains P_5^c as an induced subgraph. Hence $\lambda_3(G) \geq \lambda_3(P_5^c) = 0$. ■

THEOREM 4. *Let G be a graph on $n \geq 3$ vertices with no isolated vertices. Then*:

(1) $\lambda_{n-1}(G) \leq 0$, *with equality iff G is isomorphic to a complete bipartite graph.*

(2) *If* $-1 < \lambda_{n-1}(G) \leq 0$, *$G$ is triangle-free. Moreover, there exist no graphs such that*

$$\frac{1-\sqrt{5}}{2} < \lambda_{n-1}(G) < 0.$$

PROOF. It is easy to check that the second largest eigenvalue of every graph on three vertices is less than 0. Let $n \geq 4$. By Lemmas 3 and 9,

$$\lambda_{n-1}(G) \leq -1 - \lambda_3(G^c) \leq -1 + 1 = 0.$$

If $\lambda_{n-1}(G) = 0$, then $\lambda_3(G^c) \leq -1 + \lambda_{n-1}(G) = -1$. Then by Lemma 9, G must be bipartite, whence $\lambda_2(G) = -\lambda_{n-1}(G) = 0$ from Lemma 1(2). Since G has only positive eigenvalue, by Lemma 1(4), G is a complete bipartite graph. The converse is obvious. Part (1) is proved.

If G has a triangle, we can choose V' such that $G - V'$ is the triangle. By Lemma 1(1), $\lambda_{n-1}(G) \leq \lambda_2(G - V') \leq -1$. Suppose there exists a graph G such that $(1 - \sqrt{5})/2 < \lambda_{n-1}(G) < 0$. Then G must be triangle-free. Since G has no isolated vertices, G contains P_4 or $2K_2$ as an induced subgraph. Choose V' such that $G - V' \cong P_4$ or $2K_2$. Again by Lemma 1(1),

$$\lambda_{n-1}(G) \leq \lambda_3(G - V') = \max\left\{-1, \frac{1-\sqrt{5}}{2} = \frac{1-\sqrt{5}}{2}\right\}.$$

This contradiction completes the proof of part (2). ■

LEMMA 10. *If G^c is not a complete bipartite graph plus isolated vertices,*

$$\lambda_3(G) \geq \frac{1-\sqrt{5}}{2}.$$

PROOF. If G^c is not bipartite, by Lemma 9 we have $\lambda_3(G) \geq 0 > (1-\sqrt{5})/2$. Now assume G^c is bipartite. If G^c has two components which contain at least one edge, let uv be an edge from one component and xy an edge from the other; then u, v, x, y induce a subgraph in G isomorphic to C_4. Hence $\lambda_3(G) \geq \lambda_3(C_4) = 0$. Now suppose G^c has at most one component H with at least one edges. If H is not a complete bipartite graph, H contains P_4 as an induced subgraph. Then $\lambda_3(G) \geq \lambda_3(P_4^c) = (1-\sqrt{5})/2$. ∎

THEOREM 5. *Let G be a graph with at least three vertices. Then*

(1) $\lambda_3(G) < -1$ *iff* $G \cong P_3$;

(2) $\lambda_3(G) = -1$ *iff G^c has at least four points and G^c is isomorphic to a complete bipartite graph plus isolated vertices*;

(3) *there exist no graphs such that*

$$-1 < \lambda_3(G) < \frac{1-\sqrt{5}}{2}.$$

PROOF. (1): If $G \cong P_3, \lambda_3(G) = -\sqrt{2} < -1$. Conversely, if $\lambda_3(G) < -1$, by Lemma 9 the number n of vertices in G is less than 4. Hence $n = 3$. It is easy to check that $G \cong P_3$.

(2): If G^c is isomorphic to a complete bipartite graph plus isolated vertices, by Theorem 1 we have $\lambda_{n-1}(G^c) = 0$. By Lemma 3, $\lambda_3(G) \leq -1 + \lambda_{n-1}(G^c) = -1$. Since G^c has at least four points, by Lemma 4 we have $\lambda_3(G) \geq -1$. Hence $\lambda_3(G) = -1$.

If G^c is not isomorphic to a complete bipartite graph plus isolated vertices, by Lemma 10 we have $\lambda_3(G) \geq (1-\sqrt{5})/2 > -1$.

(3): It follows from part (2) and Lemma 10. ∎

Let $n = a + b \geq 4$. A *double star* $S(a, b)$ is a tree obtained from K_2 by joining a isolated vertices to one of the vertices of K_2 and b isolated vertices to the other. Without loss of generality, we always suppose that $1 \leq a \leq b$.

THEOREM 6. *If G^c is neither a complete bipartite graph plus isolated vertices nor a double star plus isolated vertices, then*

$$\lambda_3(G) \geq r > -0.5392,$$

where r is the second largest root of the equation $x^3 - 4x - 2 = 0$.

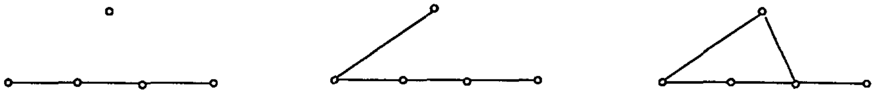

FIG. 1.

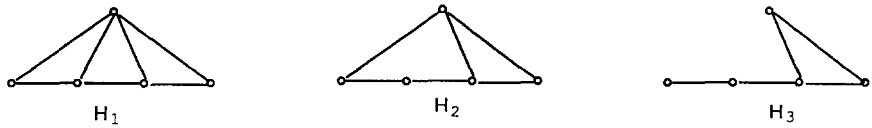

FIG. 2.

PROOF. From the proof of Lemma 10, we can suppose G^c has exactly one component G_1 which contains P_4 as an induced subgraph; the other components are isolated vertices. If G_1^c is not bipartite, by Lemma 9 we have $\lambda_3(G) \geq 0$. Now assume that G_1^c is bipartite. Let $P_4 = v_1v_2v_3v_4$. Since G_1^c is not a double star, there exists a vertex w in G^c such that w does not belong to P_4. Furthermore, G^c contains an induced subgraph isomorphic to one of the graphs in Figure 1. Consequently, G contains an induced subgraph isomorphic to one of the graphs in Figure 2. Therefore, $\lambda_3(G) \geq \min\{\lambda_3(H_1), \lambda_3(H_2), \lambda_3(H_3)\} = \lambda_3(H_3) = r > -0.539$. ■

Let D_n^* be the complement of $S(1, n-3)$. D_n^* can be obtained from $K_{n-1} - e$ by joining a new vertex to one of the vertices of degree $n-3$ in $K_{n-1} - e$.

LEMMA 11. $\chi(D_n^*, \lambda) = (\lambda + 1)^{n-4}[\lambda^4 - (n-4)\lambda^3 - (2n-5)\lambda^2 + (n-4)\lambda + n - 3]$.

PROOF. It is easy to prove that $\chi(K_n - e, \lambda) = \lambda(\lambda+1)^{n-3}[\lambda^2 - (n-3)\lambda - 2(n-2)]$. By Lemma 7,

$$\begin{aligned}
\chi(D_n^*, \lambda) &= \lambda\chi(K_{n-1} - e, \lambda) - \chi(K_{n-2}, \lambda) \\
&= \lambda^2(\lambda+1)^{n-3}[\lambda^2 - (n-3)\lambda - 2(n-2)] \\
&\quad - (\lambda - n + 3)(\lambda + 1)^{n-3} \\
&= (\lambda+1)^{n-4}[\lambda^4 + (n-4)\lambda^3 - (2n-5)\lambda^2 \\
&\qquad + (n-4)\lambda + n - 3].
\end{aligned}$$

■

LEMMA 12. *For* $n \geq 4$,

$$\frac{1-\sqrt{5}}{2} < \lambda_3(D_n^*) < -0.55495.$$

PROOF. Let $f_n(\lambda) = \lambda^4 - (n-4)\lambda^3 - (2n-5)\lambda^2 + (n-4)\lambda + n - 3$. Then $f_n(1) = -n+3, f_n(-0.55495) = 0.000018n + 0.170862$, and $f_n((1-\sqrt{5})/2) = -0.145912n + 0.583631$. If $n \geq 4$, we have

$$f_n(-\infty) > 0, \quad f_n\left(\frac{1-\sqrt{5}}{2}\right) < 0, \qquad f_n(-0.55495) > 0,$$
$$f_n(1) < 0, \qquad f_n(\infty) > 0.$$

Hence the third largest root of $f_n(\lambda)$ is in the interval $((1-\sqrt{5})/2, -0.55495)$. By Lemma 8, $\lambda_3(G_n^*)$ is equal to the third largest root of $f_n(\lambda)$. Therefore

$$\frac{1-\sqrt{5}}{2} < \lambda_3(D_n^*) \leq -0.55495. \qquad \blacksquare$$

THEOREM 7. *If G^c is not a complete bipartite graph plus isolated vertices,*

$$\lambda_3(G) \geq \lambda_3(D_n^*).$$

with equality iff $G \cong D_n^*$.

PROOF. If G^c is not a double star plus isolated vertices, then by Theorem 6 and Lemma 12, $\lambda_3(G) \geq -0.5392 > 0.55495 > \lambda_3(D_n^*)$. If G^c is a double star with at least one isolated vertex, then G^c contains an induced subgraph isomorphic to $P_4 \cup K_1$. Thus $\lambda_3(G) \geq \lambda_3(P_4 \vee K_1) = -0.4626 > -0.55495 > \lambda_3(D_n^*)$. Now suppose G^c is a double star $S(a, b)$ with $2 \leq a \leq b$. If $n \leq 6$, then by direct computation or [4], $\lambda_3(G) \geq \lambda_3(D_n^*)$. Let $n \geq 7$. G^c contain $S(2,3)$ as an induced subgraph. Hence

$$\lambda_3(G) \geq \lambda_3(S(2,3)) = -0.55134 > -0.55495 > \lambda_3(D_n^*).$$

Therefore $\lambda_3(G) \geq \lambda_3(D_n^*)$ with equality iff $G \cong D_n^*$. $\blacksquare$

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REFERENCES

1 D. Cao and H. Yuan, Graphs characterized by the second eigenvalue, to appear.
2 G. Constantine, Lower bounds on the spectra of symmetric matrices with nonnegative entries, *Linear Algebra Appl.* 65:171–178 (1985).

3 D. Cvetkovic, M. Doob, and I. Gutman, On graphs whose spectral radius does not exceed $(2+\sqrt{5})^{1/2}$, *Ars Combin.* 14:225–239 (1982).
4 D. Cvetkovic, M. Doob, and H. Sachs, *Spectra of Graphs*, Academic, New York, 1980.
5 D. Cvetkovic and P. Rowlinson, The largest eigenvalue of a graph: A survey, *Linear and Multilinear Algebra* 28:3–33 (1990).
6 M. Doob, The limit points of eigenvalues of graphs, *Linear Algebra Appl.* 114/115:659–662 (1989).
7 M. Doob, Some new results on the limit points of eigenvalues of graphs, *Abstracts Amer. Math. Soc.* 12(5):450(1991).
8 A. J. Hoffman, On limit points of spectral radii of non-negative symmetric integral matrices, in *Graph Theory and Applications*, Lecture Notes 303 (Y. Alvai, D. R. Lick, and A. T. White, Eds.), Springer-Verlag, 1972, pp. 165–172.
9 A. J. Hoffman, On limit points of the least eigenvalue of a graph, *Ars Combin.* 3:3–14 (1977).
10 A. J. Hoffman, On eigenvalues and colourings of graphs, in *Graph Theory and its Applications* (B. Harris, Ed.), Academic, 1970, pp. 78–91.
11 J. Shearer, On the distribution of the maximum eigenvalue of graphs, *Linear Algebra Appl.* 113/114:17–21 (1989).
12 H. Yuan, A bound on the spectral radius of graphs, *Linear Algebra Appl.* 108:135–139 (1988).
13 H. Yuan, Bounds of eigenvalues of a graph, *Acta. Math. Appl. Sinica* 4(2):165–168 (1988).

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